NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

CENTER FOR NEUTRON RESEARCH

SANS DATA REDUCTION AND IMAGING SOFTWARE

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1. OVERVIEW

The procedures and software that are available for displaying and processing 2D SANS data (subtracting background, converting to an absolute scale, averaging, etc.) to produce reduced 1D data in intensity vs wavenumber (**I** vs **Q**) form are described in the following sections. This section discusses some of the underlying concepts.

The raw, 2D (128 rows x 128 columns) data collected at the instrument reside in SANS user accounts in the form of individually named binary files. The format for the data file names is

XXXXXNNN.SAn_INI_AMMM,

where **XXXXX** is a 5-character sample name, **NNN** is a 3-digit user-initialized run number, and **SAn** denotes the SANS instrument where the data were collected (n=1 for the 8-meter SANS instrument on guide NG1, n=2 for the 30-meter SANS instrument on guide NG7 and n=4 for the 30-meter SANS instrument on guide NG3). **INI** denotes the user's initials and **AMMM** represents a 4-digit permanent run number used for archiving purposes. Raw data files are protected from accidental deletion at the time they are written. To delete raw data files, type **RAWDEL**, which prompts for data file name(s); the file protection is changed for all the specified files and then the files are deleted.

The 128x128 data values in the raw data files are never altered; only the file header, which contains parameters such as the beam center coordinates, detector distance, etc., can be modified (using the programs **PATCH** or **MPATCH**). For analysis the data are copied to a temporary file called a workfile named **WORK.EXT** where the file extension **EXT** is a three letter mnemonic called "data-type" that represents the logical function of the data in the workfile or indicates the processing stage they have reached. For example, data-types **SAM**, **EMP** and **BGD** identify, in turn: sample data, empty cell data, and beam blocked background data. Data-type **COR** identifies the results of combining **WORK.SAM**, **WORK.EMP** and **WORK.BGD** to produce sample data corrected for background and empty cell scattering.

The data in workfiles are processed by invoking commands that each perform a single specific operation, in some cases writing the results to a different workfile (which overwrites its prior contents). Ultimately the user invokes the command **AVERAGE** to perform either a radial, angular sector or rectangular averaging of the 2D data to reduce it to **I** vs **Q.** Azimuthal averaging can also be performed using the command **PHIAVE** to bin 2D data in a given annular region as a function of the azimuthal angle, ϕ. The averaged data are stored in individually named ASCII (text) files in a 3 column format (Q or ϕ, I, σ_I) with a 4-line header. **AVE/QSIG** creates a 6 column format containing resolution and beamstop shadowing information.

The organization of the data reduction software into dedicated, limited-function modules gives the user considerable flexibility to reduce data with a sequence of operations that best suits a particular experiment. Once determined, this sequence of commands can be stored in a separate command file (**NAME.COM**) using a text editor (e.g. EDIT). The entire sequence can then be invoked by typing @**NAME** (see Section 4).

Information on each data reduction command is available on screen by typing **HELP** followed by the command name (or just **HELP** to list the command names). A list of commands for which HELP is available can be found in Section 7.

At each stage in the data reduction process, the contents of any workfile (or raw data file) can be displayed as a color contour plot on a MACintosh. Using the MAC, a user can interactively create a mask of any portion of the 2D data field to mark those areas that are to be excluded when the data are averaged. The 2D display software is described in Section 5 and Appendix B.

Once data are reduced and saved in the **I** vs **Q** form, various types of plots (ln(I) vs Q^2, log(I) vs log(Q), etc.) can be generated on the screen and/or on a laser printer using the program **PAVE**. Note that the NG3LASER (NG7LASER) printer is the default printer at the NG3 (NG7) instrument. Linear fits to the data, to extract parameters such as the radius of gyration or **I(Q=0)**, can be carried out with the program **FIT**.

Reduced 1D data can be copied to PC or MACintosh floppy disks for storage purposes. Both raw 2D data and workfile 2D data can be converted to ASCII (text) format, using the programs **CONVERT, MCONVERT** and **ASCII**, respectively and copied to PC or MAC diskettes. The procedures for copying data to other media are described in Section 6.

2. GETTING STARTED

2.1 Logging In

Each SANS instrument has its own instrument control computer. The two 30m SANS instruments are controlled by MicroVax 4000 computers while the 8m SANS instrument is controlled by a MicroVax 3300 computer. The following associations become important in order to log onto the proper computer:

Instrument	Neutron Guide	Computer Node NAME
8m SANS	**NG1**	**SANS1**
30m NSF SANS	**NG3**	**SANS3**
30m NIST/Exxon/ U. Minn/Texaco SANS	**NG7**	**SANS2**

There are a number of SANS accounts on each computer that are assigned to users on a temporary basis (for three months) at the beginning of an experiment. To log into an assigned account on one of the MicroVaxs, use one of the following procedures.

a) From a terminal attached to the same MicroVax:

Press return and respond to the prompt for Username and Password as follows:

Username: **NGmSANSn**	(m = 3,5, or 7; n = 0,1,2,....)
Password: **??????**	(chosen by user)

NGm refers to the neutron guide on which the SANS instrument resides and **SANSn** is the assigned account number.

b) From a remote computer via internet:

Connections via internet are made using the TELNET command. The remote computer must be connected to an ethernet network and software which supports the TCPIP protocol must be installed. To connect to one of the MicroVaxs, type

TELNET	**129.6.120.12**	(to connect to RRD**SANS1**.NIST.GOV)
	129.6.120.13	(to connect to RRD**SANS2**.NIST.GOV)
	129.6.120.14	(to connect to RRD**SANS3**.NIST.GOV).

Then proceed as in a) above at the Username prompt. Be sure to use the proper network address or login will be unsuccessful. Use the TeraTerm terminal emulator program icon to connect to the MicroVax from the PCs.

c) From a MACintosh computer:

Use the program "VersaTerm-DecVT220" to select the MicroVax computer from the Sessions menu. Then use Settings/Open Connection. You will be prompted for the Username and Password.

d) From a remote computer via modem:

Connections to the NIST-wide network modem pool are made via modem by dialing **(301) 948-9720**. The modem pool supports calls at up to 9600 baud with 8 data bits and no parity. If the connection is successful, NISTnet responds with CONNECT 9600/ARQ in the case of a 9600 baud rate connection. Respond with a **<CR>** to obtain a NISTnet prompt:

Enter username>	**Username**	(any name can be used)
nistnet_m>	**con 129.6.120.nn**	(nn depends on desired MicroVax).

The number, m, in the NISTnet prompt depends upon the modem port to which the remote computer is connected. Once connected to the desired MicroVax, proceed as in a) above at the Username prompt.

Once the session is finished, hang up the modem by breaking the connection from NISTnet by typing

nistnet_m>	**lo**	(disconnects modem).

2.2 Catalog of Raw Data File Headers

To obtain a listing of the names of the data files in your account, along with most of the run information stored in the file headers, type

$**CAT [file spec]** <- file catalog program

where the brackets indicate an optional field in the command line that can be used to limit the search to a subset of file names. For example, to list the names and headers of only those files whose names start with MYDAT, type **CAT MYDAT***.

3. DATA REDUCTION

Many of the data reduction programs make use of information recorded in the raw data header at the time the data were taken. Therefore, the correct values of parameters such as the X-Y coordinates of the beam center, the detector offset, the sample transmission, etc. should be in the raw data header before proceeding with the data reduction. As described in Section 2.2, part of the raw data header can be examined with the program **CAT**. Parameter values can be viewed and edited using the programs **PATCH**, which operates on one file at a time, or **MPATCH**, which operates on multiple files. Only the raw data headers are modified, leaving the data unaffected.

Remember,

Modify incorrect parameter values in the raw data file headers with PATCH (or MPATCH) before reducing the data.

3.1 With Empirically Determined Detector Efficiency Corrections

An important step in the data reduction process involves correcting for the detector response. A data set can be corrected for non-uniformities in the detector efficiency by dividing the data, pixel-by-pixel, by the measured scattering from an isotropic scatterer such as plexiglass or water. Such corrections are optional for the ORNL-type detector (8m SANS machine) but mandatory for ILL-type detectors used on the 30 m SANS machines. Note that the detector type is listed in the file header. These corrections should be attempted only if the isotropic pattern has been counted long enough (40×10^6 total counts over the whole detector) to give good statistical precision over the entire detector. Therefore, plexiglass runs are measured periodically, by the instrument scientists, for this purpose. Plexiglass runs corrected for background and empty cell scattering are saved as **[NGnSANS0.MMMYY]PLEX_DDMMMYY_NGn.DIV** files which indicate the date the measurement was made (DDMMMYY) and the instrument used (NGn). The most recent file should be copied to **WORK.DIV** in your directory before reducing your data and to XXXXX.DIV (XXXXX being your project name) for record keeping purposes.

In case you need to redo this, follow instructions given in Fig. 2, located at the end of this manual. The data for the isotropic scatterer, Plexiglass, are first corrected for background and empty cell scattering, to create a **WORK.COR** file, then PRODIV is used to create **WORK.DIV** which represents an empirically determined detector response function. This procedure is followed only once.

Subsequently, data for all samples are corrected for background etc. and the resulting **WORK.COR** file is divided, pixel-by-pixel, by the contents of **WORK.DIV** (as shown in Fig. 3 at the end of this manual) using the command **DIVIDE COR** which generates still another workfile, **WORK.CAL**. The contents of **WORK.CAL** can then be converted to an absolute scale (described in detail in the following sections) or directly masked and averaged.

3.2 With Predetermined Detector Corrections

For the ORNL-type of 2D detector used on the 8 m SANS instrument the detector response gradually becomes nonlinear toward the edges. In the data reduction scheme described here, and shown schematically in Fig.1 (which can be found at the end of this manual), predetermined

correction factors are automatically applied to the data. These correction factors are based on a smooth analytic function that accurately describes the detector response except for a few rows and columns at the edges where the response is highly nonlinear. The edges of the detector should be masked (see Section 5.1 for details) so that they do not contribute to the determination of **I** vs **Q**.

3.3 Command Sequences for Data Reduction

The most commonly used sequence of data reduction steps is shown schematically in Fig. 3. The first program module, **ADD**, 1) moves raw data to either the **SAM, EMP,** or **BGD** workfiles, 2) applies the empirical detector correction factors, and 3) normalizes the data to a fixed number of incident neutrons (corresponding to a monitor count of 10^8 counts) to facilitate comparisons between data sets. After **ADD** has been used to fill the **SAM**, **EMP** and **BGD** workfiles, the program **CORRECT** is invoked to correct the data for background and empty cell scattering according to the algorithm

$$\mathbf{COR = (SAM - BGD) - [T_{sam}/T_{emp}](EMP - BGD)}$$

where T_{sam} is the transmission of the sample and T_{emp} is that of the empty cell. Note that T_{sam} and T_{emp} are taken with respect to the empty beam. Thus, if no cell is used (i.e., empty beam condition), T_{emp} = 1.0. The results of this operation are stored in another workfile, **WORK.COR**. Upon applying detector corrections **DIV COR**, the file **WORK.CAL** is obtained.

At this point the corrected data may be reduced to **I** vs **Q** by running the program **AVERAGE**, or converted to an absolute intensity scale (**I(Q) ->d**Σ**/d**Ω in units of cm^{-1}) using the program **ABSOLUTE** and then averaged. In order to use **ABSOLUTE**, the scattering from a standard sample must have been measured under the same experimental conditions and reduced to obtain **I(Q=0)**, which **ABSOLUTE** needs to compute. (See Section 3.5 for details.)

The last step before averaging the data to reduce it to **I** vs **Q** form is to run the program **MASK** which has the effect of marking, or masking, specific pixels in the 2D data field that are to be ignored in the subsequent averaging process. The mask is generated on the MAC by interactively marking the color image of a data set (using the display software described in Section 5). In order to transfer a mask (created on the MAC) to the MicroVax computer, use **GETMASK**. This will save the mask on the MicroVax with the same name as on the MAC. Remember to copy this file to **WORK.MSK** before reducing your data.

Remember,

Mask workfiles immediately prior to averaging to produce I vs Q.

The program **AVERAGE** performs either a radial, angular sector or rectangular averaging (ignoring all masked pixels) of the 2D data field to reduce it to **I** vs **Q**. The averaged data are stored in individually named ASCII (text) files in 3 columns (Q, I and σ_I separated by spaces) with a 4-line header. Use **AVE/QSIG** to create a 6 column format containing resolution and beamstop shadowing information. Data that have been converted to an absolute scale are, after

averaging, stored in a file with the extension **.ABS**; otherwise, if **ABSOLUTE** has not been run, the results are stored in a file with the extension **.AVE**.

The diagram in Fig. 3 represents the most common data reduction scheme, but the user is free to construct an alternative one. For example, to subtract data for a "blank" from that for a sample and average the difference, use **ADD** to deposit the sample data in **WORK.SAM** and the blank data in **WORK.EMP** (or **WORK.BGD**). Then use **SUB** which subtracts data from the two workfiles (**SAM** and **EMP**) and stores the difference in another workfile, **WORK.SUB**. Finally, mask **WORK.SUB** (by typing **MASK SUB**, for example) and run **AVERAGE**.

Note that a different type of averaging can be performed using the program **PHIAVE**, which bins 2D data in an annular region as a function of the azimuthal angle, ϕ. **PHIAVE** prompts for the Q value at the center of the annular region (corresponding to a peak for example), which can be found by radially averaging the data first using **AVERAGE**. The azimuthally averaged data are also stored in individually named ASCII files in 3 columns (ϕ, I and σ_I separated by spaces) with a 4-line header. The extensions, **.ABS**; and **.AVE**, are used in the same manner as described above.

Processing several data sets in the same way can be expedited by storing the necessary sequence of commands in a file (**NAME.COM**) using a text editor (e.g. EDIT). The sequence of commands can then be invoked with a single command (**@NAME**) (see Section 4 for details).

3.4 "Multiple" Data Reduction Commands

A short description of the SANS commands that can be used to reduce a series of data files (with the same project name and sequential run numbers) follows.

MPATCH to make identical corrections in multiple raw data file headers
MVIEW to send a series of files from the MicroVax to the MAC computers
MXFER to send a series of files from the MicroVax to the IMAGE2.SANS file on the MAC
MCONVERT to convert a series of binary raw data files to ASCII (text) format
MRED to reduce a series of raw data files without subtracting background and without absolute rescaling (ADD SAM, DIV SAM, MASK CAL, AVE CAL)
MRED_COR to reduce a series of data files with background subtraction and without absolute rescaling (ADD EMP, ADD BGD, ADD SAM, COR, DIV COR, MASK CAL, AVE CAL)
MRED_ABS to reduce a series of data files without background subtraction and with absolute rescaling (ADD SAM, DIV SAM, ABS CAL, MASK ABS, AVE ABS)
MRED_COR_ABS to reduce a series of data files with background subtraction and with the absolute rescaling (ADD EMP, ADD BGD, ADD SAM, COR, DIV COR, ABS CAL, MASK ABS, AVE ABS)
MRED_KAP to reduce a series of data files with background subtraction and using the direct beam flux measurement method for absolute intensity scaling
MSUM sums the counts in a rectangular region of a sequential series of raw data files; prompts for range of rows and columns to sum over; used primarily for computing sample transmission

All of these commands are entered from the keyboard (type MRED for example). As input, most of them require a project name, first run number, and last run number. Some of them also require filenames for the EMP and BGD runs, absolute standard information, etc. Note that most of these commands generate a batch file (called JUNK.COM) which is then executed.

3.5 Converting Data to an Absolute Scale

Data are placed on an absolute scale by measuring a standard sample under the same spectrometer conditions as those used to acquire the data. The **ABSOLUTE** program is used to convert the 2D data to an absolute intensity scale.

The scattered intensity **I(Q)** reported by the **AVERAGE** program is related to the absolute cross-section **d**Σ**(Q)/d**Ω by the expression:

$$I(Q) = \phi\, A\, d\, T\, (d\Sigma(Q)/d\Omega)\, \Delta\Omega\, \varepsilon\, t,$$

where ϕ = flux on the sample,
A = sample area,
d = sample thickness,
T = measured sample transmission,
$\Delta\Omega$ = solid angle subtended by one pixel of the detector,
ε = detector efficiency, and
t = effective counting time, which was renormalized (in the program ADD) to give 10^8 monitor counts (MON).

By dividing this expression for the data by a similar expression for the standard sample, **ABSOLUTE** calculates the absolute cross-section for the data from:

$$\frac{d\Sigma(Q)}{d\Omega} = \frac{I(Q)}{I_S(0)} \frac{MON_S}{MON} \frac{d_S}{d} \frac{T_S}{T} \frac{d\Sigma_S(0)}{d\Omega}$$

where: $I_S(0)$ = measured intensity of the standard sample at Q=0,
d_S = thickness of the standard sample and
T_S = measured transmission of the standard sample (which is wavelength dependent).
Note that if I(Q) and $I_S(Q)$ are from radially averaged work files then MON_S=MON.

ABSOLUTE reads the values of T_S, d_S, $I_S(0)$ for the default monitor count, and $d\Sigma_S(0)/d\Omega$ from the file ABSPRAM.DAT. If the current values are incorrect, they may be changed before proceeding. Data which have been placed on an absolute scale will have the extension **.ABS** after they are averaged.

The appropriate standard sample is selected, for the most part, based upon the Q-range in which the measurement is being made. The range of Q values applicable for each standard sample is given in Table1.

3.5.1 Silica Standards

The silica standard samples should be used under conditions where the scattering is weak enough such that an attenuator does not have to be used to reduce the total counts on the detector and where the Q-range from **0.01 Å^{-1} to 0.025 Å^{-1}** for Silica B or **0.02 Å^{-1} to 0.04 Å^{-1}** for Silica A is covered. Thus, the silica standards should be used at longer wavelengths on the 8m SANS instrument and at intermediate detector distances on the 30m SANS instrument.

The absolute cross-sections of the silica standards have been measured using a direct method without reference to another sample. The absolute beam current was determined by calibrating the pinhole area of a set of small apertures, which were used as attenuators, and then measuring the attenuated beam intensity. The absolute cross-section is then given by

$$\frac{d\Sigma(Q)}{d\Omega} = \frac{j_{beam}\,\varepsilon_D}{T_{atten}}\,\frac{MCR}{1x10^8\,\Delta\Omega}\,\frac{I(Q)}{d\;T_s}$$

where $j_{beam}\varepsilon_D/T_{atten}$ is the detected beam current measured by the SANS detector corrected for attenuation, MCR is the monitor count rate (the factor $1x10^8$/MCR is for the monitor count rescaling completed in the ADD program), $\Delta\Omega_{pixel}$ is the solid angle subtended by a pixel, d_S is the sample thickness and T_S is the sample transmission. The measured absolute cross-sections for the A and B silica standards, along with the sample thickness and applicable Q-ranges for each can be found in Table 1 at the end of this manual.

Before invoking **ABSOLUTE**, the 2D data from the silica standard sample must be reduced and averaged as described in Section 3.3. Then, $\mathbf{I_S(0)}$ is found by fitting the averaged data (using the program **FIT**) in the appropriate Q-range from Table 1, where the scattering curve can be accurately extrapolated to Q = 0. The radius of gyration, R_g, obtained from the Guinier fit is also listed in Table 1. The **ABSOLUTE** program requires the fitted value, $\mathbf{I_S(0)}$, the absolute intensity, $\mathbf{d\Sigma_S(0)/d\Omega}$, the standard sample thickness, $\mathbf{d_S}$ and its transmission, $\mathbf{T_S}$.

3.5.2 Water Standard

The scattering from 1mm of water is generally used in place of the silica standard samples under conditions where the silica sample scatters too strongly or where $\mathbf{Q_{min}>0.02Å^{-1}}$. Thus, the water sample should be used for shorter wavelength measurements on the 8m SANS and for short detector distances on the 30m SANS instruments.

Before invoking **ABSOLUTE**, the 2D data from the 1mm water sample must be reduced and averaged as described in Section 3.3. The mean value for the intensity of the water sample, $\mathbf{I_{water}(Q)}$, replaces $\mathbf{I_S(0)}$ and should be determined over the Q-range where the intensity is approximately flat on an I(Q) vs Q plot. This should include almost the entire measured Q-range except for the smallest Q values, where some parasitic scattering may be seen, and perhaps the last few data points, where masking effects make the data noisy.

When using **ABSOLUTE**, the measured transmission of the water sample, $\mathbf{T_S}$, and its thickness, $\mathbf{d_S=0.1cm}$, should be used. The measured values of $\mathbf{d\Sigma_S(Q)/d\Omega}$ are listed as a function of neutron wavelength in Table 2 at the end of this manual. Due to the uncertainties in the values of the cross section for water, water is recommended only when no other standard can be used.

3.5.3 Polystyrene Standards

The absolute intensities of the AS, B and C polystyrene standards have been determined by the direct neutron flux measurement method also used for the silica standards. The absolute cross-

sections, along with the sample thickness and applicable Q-ranges for each can be found in Table 1 at the end of this manual. The polystyrene standards are well-suited for measurement in the intermediate to long configurations of the 30m SANS instruments.

Before invoking **ABSOLUTE**, the 2D data from the polystyrene standards must be reduced and averaged as described in Section 3.3. Then $\mathbf{I_S(0)}$ is found by nonlinear fitting the averaged data to the RPA equation (see Appendix A) using the program **FIT/RPA**. A scale factor and the monomer segment length, **b**, are varied in the fit. The fixed parameters used by **FIT/RPA** can be found in Table 3 at the end of this manual. A wavelength-dependent correction to $\mathbf{I_S(0)}$ for multiple scattering is automatically made in **FIT/RPA**. The transmission of the standards, $\mathbf{T_S}$, measured with respect to the empty beam, and their thicknesses are also required by **ABSOLUTE**.

3.5.4 Direct Beam Flux Measurement

Another method for rescaling data to an absolute intensity consists in a direct measurement of the beam flux at the sample using the area detector. This measurement is similar to the empty beam measurement when measuring transmissions (move attenuator in and the beam stop out). This method is more complicated but could be a useful check independent of standard samples. In order to implement this method, the quantity $K= \phi A \Delta\Omega \varepsilon t$ must be calculated . Here ϕ is the flux on the sample, A is the sample area, $\Delta\Omega$ is the solid angle subtended by one pixel of the detector, ε is the detector efficiency, and t is the effective counting time. Then ABS is run with the following parameters:

1) T_{sample} 2) d_{sample} (cm) 3) Trans=1.0 4) Thick=1.0 (cm) 5) I(0)=K 6) 1.0

K is calculated as follows: $\phi A \varepsilon$ is the total (empty beam transmisssion) detector counts per unit time/attenuation factor at the used wavelength, t is the counting time $x10^8$/MCR, and $\Delta\Omega$ is equal to (0.5 cm/sample-to-detector distance in cm)^2.

The program **MRED_KAP** is easier to use because it obtains this required information from the direct beam measurement file and calculates K internally.

4. DATA REDUCTION WITH COMMAND FILES

4.1 Use of Command Files

When several data sets are to be processed in the same way, typing (and the chances of mistyping) can be minimized by storing the sequence of data reduction commands in a separate file with the extension **.COM,** e.g. **NAME.COM**. The entire sequence of commands can then be executed by typing **@NAME**. Any text editor that generates an ASCII file, such as the MicroVax **EDIT** command, can be used to construct the command file.

A copy of a prototype command file, **REDUCE.COM**, containing the sequence of commands listed below, is available in each SANS account on the MicroVaxs and is reproduced below. If you wish to modify this file for your own use, please first use the **COPY** command to make a copy of the file with a new name.

REDUCE.COM
$SET VERIFY **<- causes each subsequent line**
$TT **to be displayed at the terminal**
$ADD SAM
$CORRECT
N
N
$ABSOLUTE COR **<-blank line required below**

$MASK ABS
$TT
$AVERAGE ABS
$SET NOVERIFY **<- cancel verify mode**

In the above example, note that each command line starts with **$**, the MicroVax VMS prompt symbol. Note also that if a command requires a response that is the same for each data set, the response can be included in the command file as is the case for the commands **CORRECT** and **ABSOLUTE** in the above example. If, on the other hand, the response to a command changes each time the command file is run, then the command must be preceded by the line **$TT** (the symbol TT stands for DEFINE/USER_MODE SYS$INPUT SYS$COMMAND) which causes the file to wait for input from the keyboard. This is the case with the commands **ADD** and **AVERAGE** in the above example which require the name of the input and output data files, respectively. The names of these data files can be placed in the command procedure so that input from the keyboard, and thus the command line, **$TT**, is not necessary. In such cases where no user intervention is required to run the command procedure, it can be run in the background as a batch job by typing **SUBMIT NAME.COM**. In this case, a record of the program execution, including the program prompts and the responses obtained from the command file, is kept in the file **NAME.LOG**.

Another command file **MREDUCE.COM** allows the reduction of a set of files (that have the same project name) using the same set of commands. Here also, the command sequence can be modified by editing **MREDUCE.COM**.

4.2 Editor Features on the MicroVax

Some useful editing features on the MicroVax are included here. To start editing, type **EDIT NAME.COM**, then use the numeric keyboard block located to your right.

>> To select a block of words or lines, press the period (**.**) key, then the arrow keys.
>> To remove (cut) the selected block, use the **6** key.
>> To paste the block that has been removed (cut), press the **PF1** then the **6** keys sequentially.
>> To find a word, press **PF1** then **ENTER** followed by the **PF3** key. To find the next word, press
>> To delete a line, press the **PF4** key. To delete a character, press the comma (**,**) key, to delete to the end of the line press the **PF1** then the **2** keys.
>> To go to the top of the file, press the **PF1** and **5** keys.
>> To go to the bottom of the file, press the **PF1** and **4** keys.
>> To select the “forward” feature, press the **5** key, to select the “backward” feature, press the **4** key. These are useful when searching, replacing, etc.
>> To find a string of characters, then replace it by another string, first “find” the

old string, then create a “paste” with the new string, then keys **PF1** then **ENTER** will do the “find/replace” in one swoop.

>> Most of the above features can be performed a number **n** of times automatically by pressing the **PF1** then **7** then **n** keys sequentially before pressing the key sequence for the feature desired.

>> To define a **MACRO key** that would execute a sequence of commands when pressed, do the following: Press **Control K**, then the key to be defined (Choose one of the **F9-F20** keys), then the sequence of commands in parenthesis, then a period followed by **ENTER** to end the definition of the function. This is a powerful and useful feature. One can for example define the **F9** key to “find” a specific string, “replace” it by another, move to the next line (down arrow), move to the right two character positions (right arrow), insert another string, etc. In order to execute this sequence, press the defined **MACRO key** followed by **ENTER**.

To exit the editor, press the **PF1** and **7** keys, then answer the command prompt by **EXIT** to save the changes that were made or by **QUIT** to quit without saving the changes, then press the **ENTER** (not the **RETURN**) key.

Note that when using a MAC or the PC running TeraTerm as terminal emulator, the alphanumeric keys are as follows:

Alphanumeric Keyboard:

PF1	PF2	PF3	PF4
7	8	9	-
4	5	6	,
1	2	3	ENTER
0	0	.	ENTER

5. DATA DISPLAY SOFTWARE

5.1 2D Data

Color contour plots of either raw data files or workfiles can be displayed and printed using the MACs at each SANS instrument or the MACs (node names MACCX1, MACCX2, MACSI1, MACSI2, MACPPC, etc.) in the computer terminal room. The procedure involves two steps, 1) transferring a data file from the MicroVax to the MAC, and 2) invoking the program **SANS Image** that runs on the MAC to display the data. These two steps are described in detail below.

1) Log on to your SANS account on the appropriate MicroVax from the MAC (or from another terminal). To log on, use the mouse to position the cursor (an arrow) over the name SANSn (n=1, 2, or 3) in the window named VersaTerm and press the mouse button twice quickly (double click). If the VersaTerm window is not present, double click on the hard disk icon, labeled MACII, in the upper right hand corner of the screen ("desktop"), then use the vertical scroll bar until you find it. Pull the Session/ NGnSANS, then the Settings/Open Connection menus to establish a network link between the MAC and the MicroVax and to open a window on the MAC screen where you can log onto the MicroVax just as you would if you were at a dedicated terminal (see Section 2.1). After logging on to your SANS account on the MicroVax, type

$VIEW

to run a program that will prompt you for the name of the raw data file you want to display (view workfiles with the **VIEW/WORK** program) and also allow you to select how you want the data displayed (e.g. on a linear or logarithmic color scale, etc.). When your choices are made, **VIEW** will map the data to values from 0 to 255 and send the mapped data values to the MAC where they will be stored in a file with the same name in a folder named SANSNG3, SANSNG5 or SANSNG7, depending upon the SANS instrument used to take the data.

NOTE: Before transferring files to the MAC, you may wish to "clean up" the SANSNGn folder by deleting the files left by previous users. One way to accomplish this is to open the SANSNGn folder by double-clicking on its icon. (If this doesn't open the folder, make sure MACII is the active window by clicking on its title bar.) Then position the cursor over the EDIT menu and click on the command SELECT ALL. (You can "de-select" individual files you wish to keep by clicking on them while holding down the SHIFT button.) After selecting the files, hold down the mouse button, while positioning the mouse on any one of the selected files, and "drag" the files into the TRASH at the lower right-hand side of the screen. The trash can will become highlighted when you have positioned the mouse correctly. Upon releasing the mouse button, the trash can will bulge. Select **EMPTY TRASH** from the SPECIAL menu to delete the files. (You can retrieve any

file out of the TRASH folder before emptying the trash. Double click on the trash can icon to open the folder. Select the file you wish to retrieve and drag it out of the trash.)

2a) If the program **SANS Image** is currently active (one way to check is to cycle through the icons for the programs that are active by clicking on the small icon in the far right-hand corner of the main menu bar), select the command **IMPORT SANS** from the FILE MENU. A standard MAC file selection box appears on the screen. Use the vertical scroll bar to find the SANSNGn folder and double click on the folder name (or single click on the folder name to select it and then click on the OPEN button) to list the individual files stored in the folder. Once again scroll through the list to find the file you want to display and double-click on its name to import the data into **SANS Image**.

2b) If the program **SANS Image** is not currently active, simply double click on the name of the file you want to display (which is stored in the SANSNGn folder.)

Once an image of a data file is displayed, any of the "tools" shown on the left-hand side of the screen can be used to modify the image. A diagram of the tool window as well as a brief description of each tool is given in Appendix B. The X-Y pixel numbers corresponding to the cursor location and the mapped value (0-255) for the corresponding data point can be found in the RESULTS window at the bottom left of the screen. The pixels on the MAC are 1-128 which corresponds to X-Y coordinates for the raw data. The actual intensity value is also shown in parenthesis (Value=).

The color look-up table (LUT) defines the default color palette for the **SANS IMAGE** program. Click in the LUT window with any of the drawing tools (described in Appendix B) to pick up a new drawing (foreground) color. Click in the LUT window with the eraser to pick up a new background color.

The color palette can be moved and/or stretched (shrunk) using the LUT tool. Click and drag near the bottom of the palette to move it within the LUT. Click and drag near the top of the palette to stretch or shrink it. The LUT can be edited, if desired, by double-clicking on a color with the eyedropper tool.

Information can be obtained on-line using Balloon Help by selecting “Show Balloons” found under the AppleGuide menu at the upper right of the menu bar. A few of the operations that Image provides that are particularly useful for SANS data are described in Appendix B.

SPYGLASS Transform (installed on a few MACs) can also be used to visualize SANS data (publication quality contour maps, etc). A one-page summary on how to use SPYGLASS Transform can be found in Appendix C.

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5.1.1 Masking Data

Several of the drawing tools available in **SANS IMAGE** can be used interactively to create an arbitrary data mask that delineates those regions of the 2D data field that are to be excluded when the data are reduced to **I** vs **Q** form. Once created, the data mask can be transferred to the MicroVax where it is stored in the file **WORK.MSK** that is used in processing each data set (see Section 3).

A data mask is denoted by a particular color that appears near the bottom of the color bar (or LUT for look-up table) and is labeled: mask. To mask the border regions of a data image, for example, click on the paintbrush tool and then click on the mask color in the LUT. Position the cursor (now shown as a circle) near one corner of the image, then hold down the mouse button while moving the cursor over the region to be masked (pressing the SHIFT key at the same time restricts the cursor to move only horizontally or vertically). To mask a circular region, click on the oval shaped selection tool, then click and drag (i.e. hold button down) the cursor near the region to be masked (holding the SHIFT key down at the same time forces the selected region to be circular). Release the mouse button when the circular area has the desired size. At this point, while the outline of the selected area is flashing black and white, you can change the size of the circle by clicking anywhere outside it, which cancels the selection, and starting over. Or you can reposition the circle by clicking inside the circle and dragging it to a new location (or use the arrow keys to "nudge" the selection one pixel at a time). When you are satisfied with the size and location of the circle, select **FILL** from the EDIT menu to color the circle (if the fill color is not the same as the masking color, click on the word mask near the bottom of the color bar). Finally, click anywhere outside the circle to erase the tool outline.

Once a portion of a data image has been masked, the mask can be saved to a file on the MAC by using the **SAVE MASK** command from the FILE menu (be sure that the mask to be saved is in the currently "active" window - to make a window active, click on its title bar). A previously saved mask can be displayed in its own window (as well as a window titled MASK) by using the **OPEN MASK** command. Once displayed in the window titled MASK, a mask can be superimposed on an active data window with the **APPLY MASK** command found under the FILE menu.

To transfer a saved mask file from the MAC to the MicroVax for use in reducing data, type

$GETMASK [node] (node = MAC node name),

which is run from the MicroVax (not the MAC). If the node is left blank, **GETMASK** will prompt for the MAC node name. The default node is MACCX1, located in the terminal room. **GETMASK** will list all of the mask files currently in the SANSNGn folder on the MAC and prompt you to select one for transfer to the MicroVax where it will reside with the same filename. Copy this mask file to **WORK.MSK** (this overwrites the previous contents of **WORK.MSK**) before using the **MASK** command.

Appropriate default mask files, usually called **BORDER.MSK** or a variation thereof, which mask the edges of the detector only are located in the SANSNGn folders. Often, one these masks is sufficient and may be used in lieu of creating a new mask on the MAC.

5.1.2 Intensity Profiles

On the MAC, intensity profiles can be generated using the density profile tool (see Appendix B), which displays a plot of the scaled data values along an arbitrary line. After selecting the density profile tool, place the cursor at the position where you wish to start the profile. While holding down the mouse button, move the cursor until the line defining the region of the density profile is in the desired position. When you release the mouse button, an intensity profile plot will appear in the PLOT window.

The plot options can be altered by selecting the **PROFILE PLOT OPTIONS** command from the OPTIONS window. Double-clicking on the density profile tool also brings up the Profile Plot Option dialog box.

5.1.3 Locating the Beam Center

The X-Y coordinates of the center of the data can be located using the wand (auto-outline) tool (see Appendix B). To find the data (or beam) center,

1) If measuring on the real-time image, IMAGE1.SANS, choose **PAUSE UPDATING** from the OPTIONS menu
2) Double-click on the wand tool or select **DENSITY SLICE** from the OPTIONS menu to enable density slicing. A selection region, which can be moved, shrunk or stretched in the same manner as the entire color palette, appears in a red color within the LUT. Manipulate the selection region in the LUT window until the highlighted region of the data corresponds to the intensity coun tours surrounding the data center. Only the highlighted pixels will be included in the measurement
3) Select **MEASURE** from the ANALYZE menu.
4) Read the X-Y coordinates by selecting SHOW RESULTS from the ANALYZE menu.
5) Choose **RESUME UPDATING** from the OPTIONS menu if updating was paused.

5.2 1D Data

Once the data have been reduced to 1D **I** vs **Q** form, **PAVE** can be used to produce plots on the screen and/or the laser printer (the NG3LASER printer close to the NG3 instrument (NG7LASER close to the NG7 instrument) is the default printer. Typing **LASERJET** selects the LaserJet-5si printer in the computer room. **PAVE** presents the same plotting options that are available in **AVERAGE** (I vs Q, ln(I) vs Q^2, log(I) vs log(Q), etc.). Error bars are included. Note that on the PCs used as terminals to connect to the MicroVax computer, type PC when prompted to ENTER TERMINAL TYPE inside the **PAVE** program.

FIT performs a weighted least-squares fit of a straight line to averaged data. Before fitting, the data are recast into one of the following forms:

1)log(I) vs log(Q)
2)ln(I) vs Q^2
3)1/I vs Q^2
4)I^a vs Q^b — a and b need not be
5)IQ^a vs Q^b — integer values
6)$1/\sqrt{I}$ vs Q^2
7)ln(IQ) vs Q^2
8)ln(IQ^2) vs Q^2.

The results are reported to the screen and may also be printed and plotted on the laser printer (NG3LASER or NG7LASER at the instruments). **FIT** is useful for determining the radius of gyration from ln(I) vs Q^2 plots, the Porod constant, S, from IQ^4 vs Q^4 plots, the power law slope from log(I) vs log(Q) plots, etc.

6. COPYING DATA TO OTHER MEDIA

Both 2-D and 1-D (averaged) data can be saved on PC floppy disks. The 2-D data must first be converted from binary to ASCII (text) format using either the program **CONVERT**, for raw data or **ASCII** (text) for work file data (see sections 6.2 and 6.3).

SANS data images and masks (in the SANS IMAGE format) can also be transferred from a remote Macintosh to our facilities Macs using standard FTP programs (such as FETCH). The IP addresses of Macs at the 30 m SANS instruments are:

129.6.120.54 for the MACNG7
129.6.120.55 for the MACNG3.

When connecting-in, the Macs user ID is USER and the password is NEUTRON on both instruments.

6.1 Averaged (1D) Data

To save averaged data files on **PC floppies or on a zip drive** at the instrument (using the PC running TeraTerm):

1) Put a PC floppy (1.4 Meg) or a 100 Meg zip drive.
2) Open the Ws_FTP Program, then open a window into your account on the MicroVax.
3) Change to the right subdirectory by clicking on that directory name.
4) To transfer files from the MicroVax to the PC drive, selct the files then click the left arrow. You can transfer only ASCII (text) files such as averaged SANS data, and only about 10 files at a time (not to crash the FTP program on the MicroVax). In order to select blocks of files at a time, it is recommended to copy the ASCII files to another MicroVax subdirectory containing only these files and do the transfer from that subdirectory.
5) To exit ftp, click close.

To save averaged data on **MAC floppy disks**, do the following:

1) Put a FORMATTED floppy diskette into the disk drive on one of the MACs in the computer terminal room.
2) Open the **VersaTerm** communication program, if not already running, by double clicking on the VersaTerm icon. If the icon is not on the desktop, it can be found in the Applications Folder on the hard disk labeled MACII.
3) From the VersaTerm File Menu, select **Config... [FTP Client]**. From the list of TCP/IP Hosts presented, select the SANS computer, SANSn, where your data are stored. Also enter your account name, e.g. NGnSANSxx, and password in the Username and Password boxes. Then click OKAY.
4) Again from the VersaTerm File Menu, select **Receive File**. VersaTerm will then open a window displaying the file names in your account on SANSn. Click on a file name to select it for transfer. Multiple files can be selected for transfer by holding down the SHIFT key when clicking on individual file names. When the files to be transferred have been selected, click on the RECEIVE button (make sure that file type is Text/ASCII not Binary). You will then see a window that allows you to specify the transfer destination. Select your floppy diskette as the destination. Click SAVE to initiate the transfer.
5) When the transfer(s) are complete, click DONE.
6) Eject the floppy diskette from the disk drive by dragging the floppy

disk icon to the trash can.

6.2 Raw (2D) Data

Once converted to ASCII form, 2D raw data can be saved to PC or MAC floppy disks in the same way as averaged data. In order to convert the data in **.SAn_INI_A000** files from binary to ASCII form, use the program **CONVERT** for one file and **MCONVERT** for a series of files under the same project name. Converted files have the same name with the extension **.ASC**. Follow the procedure outlined in Section 6.1 above to transfer the **.ASC** files. Storage of binary **.SAn_INI_A000** files on PC or MAC floppies is not recommended since they will not necessarily transfer properly going from MicroVax to PC or MAC and back. If it is necessary to retrieve a stored 2D file for further data analysis, it can be converted back to binary form using the program **UNCONV**.

6.3 Workfile (2D) Data

Once converted to ASCII form, workfile data can be saved to PC or MAC floppy disks in the same way as averaged data. In order to convert the data in **WORK.XXX** files from binary to ASCII form, use the program **ASCII** The name of the converted file is chosen by the user. The **ASCII** program has several options which write the data in different formats. For more information, type **HELP ASCII**. Follow the procedure outlined in Section 6.1 above to transfer the converted files.

7. SANS HELP UTILITY

7.1 Command List

On-line help is available for any of the SANS commands by typing **HELP**. Once you are in the HELP utility, type the command name at the **?** prompt to get information on that command. Type @**VAX** at the **?** prompt in order to obtain a list of additional native MicroVax commands for which help is available. To exit the HELP utility, type successive carriage returns at the **?** prompt until the standard MicroVax prompt reappears.

A listing of SANS commands follows:

ABSOLUTE	ADD	ASCII	AVERAGE	CAT	
COMBINE	CONCENTER	CONTRAST	CONVERT^{+}	COPY	
CORRECT	CMBN	DATAPLOT	DATATYPES	DELETE	
DEPOSIT	DIRECTORY	DIVIDE	EDIT	FINGER	
FIT	FIT/RPA	FORTRAN	FTP	GETMASK	
HELP	INSPECT	INSTRUCTIONS	LASER	LINK	
LOGOUT	MASK	MORPLT	MPATCH	MVIEW	
MXFER	NORMALIZE	NSORT	PATCH	PAVE	
PHIAVE	PRINT PRODIV	PURGE	QSCALES		RAWDEL
RECENTER	REFORMAT	RELABEL	RENAME	RESCALE	
RESMOD	RUN	SASCALC	SIMWORK	SMEAR	

STOR*	SUB	SUBMIT	SUM	SWAP
TAP	TELL	TELNET	TEMPMON	TOTAL
TXL	VIEW			

+CONVERT_UNCONV
*STOR_UNSTOR

7.2 Command Information

A short description of some of the most frequently used SANS data reduction commands follows. Use

ABSOLUTE to place data on an absolute scale
ADD to move raw data to **SAM**, **EMP**, or **BGD** workfiles
ASCII to convert binary workfile data to ASCII format
AVERAGE to reduce 2D raw data to 1D **I** vs **Q** data
AVE_NOTRANS does the averaging without the solid angle correction to the transmission (non-negligible only at short sample-detector distances)
CAT to get a catalog of raw data file headers
CONVERT to convert binary raw data files to ASCII format
CORRECT to correct data for background and empty cell scattering
CMBN to combine (add/subtract) two averaged files, and subtract background from them
DIVIDE to correct for non-uniformities in the detector efficiency
FIT to perform a linear least-squares fit to averaged data
FIT/RPA to perform a non-linear fit to the RPA equation
FIT/SMEAR to fit data to models including instrumental smearing effects
GETMASK to transfer a mask file from the MACintosh to the **MSK** workfile
INSPECT to examine workfile or raw data file contents
MASK to imprint the current mask on a workfile
MCONVERT to convert a series of binary raw data files to ASCII format
MPATCH to make identical corrections in multiple raw data file headers
MRED to reduce a series of raw data files
MRED_ABS to reduce a series of raw data files with absolute intensity rescaling
MRED_COR to reduce a series of corrected data files
MRED_COR_ABS to reduce a series of data files runs into an absolute intensity scale
MRED_KAP to reduce a series of data files runs to an absolute scale using the direct beam method
MSUM to sum the counts in a rectangular region of a sequential series of raw data files
MVIEW to send a series of files from the MicroVax to the MACintosh computers
MXFER to send a series of files from the MicroVax to the IMAGE2.SANS file on the MACintosh
NORMALIZE to change a workfile monitor count
NSORT to inter-normalize and sort two averaged data files
PATCH to make corrections in raw data file headers
PAVE to plot averaged data on the screen or laser printer
PHIAVE to plot and store 2D data in an annular region as a function of the azimuthal angle ϕ
PRODIV to scale the data in the **COR** workfile to average 1 count/pixel and put the result in the **DIV** workfile
RECENTER to change the X-Y coordinates of the beam center in a workfile header
RELABEL to replace the current label in a workfile header
RESCALE to rescale workfile data

SMEAR to compute instrumental smearing to selected model scattering functions
STOR to copy a workfile to temporary storage in the **STO** workfile
SUB to subtract two workfiles and put the results in the **SUB** workfile
SUM to obtain the total count values in a specified X-Y region of the data field
PRINT_LOG to obtain a hard copy (on the default printer) of the SANS Log file
VIEW to display a color image of a raw data file on the MACintosh
VIEW/WORK to display a color image of a workfile on the MACintosh.

8. THE NIST SANS INTERNET HOMEPAGE http://rrdjazz.nist.gov/sans.html

This homepage gathers useful information for users. It contains:

- **NIST SANS Instruments** describes the two 30m NIST-SANS instruments
- **NIST SANS Schedules** contains the online schedules (for the NIST SANS instruments)
- **NIST SANS Scientists** contains coordinates of SANS scientists (local contacts).
- **Information to SANS Users** includes: How to Obtain Beam Time, How to Gain Access to the Neutron Scattering Facilities, How to Reserve Dosimeters, Local Area Hotels, Maps, Airport Shuttles, etc.
- **SANS Manuals/Tutorials** available as Adobe Acrobat files. The Adobe Reader (freeware) is required.
- **Drawings/Equipment Pictures/SANS Images** contains drawings of SANS cells and sample environments, etc.
- **SANS Image Preview** to access SANS images on the internet. To view some of your data files (upto 20 of them) on the internet, type COPY XXXXXNNN.SA* IMAGEn from a Microvax terminal (Here XXXXXNNN.SA* is the raw data filename and n=1 to 20).

The “Information to SANS Users” page contains an item “How to Obtain Neutron Beam Time” which contains a link to the **Web Proposal Form** (http://rrdjazz.nist.gov/howprop.html).

An internet browser (Netscape) is available on the MACs and on the PCs running Windows.

9. MAC AND PC APPLICATION SOFTWARES AVAILABLE

The following application softwares have been installed on the MACs.

On the Desktop:

>> SANS Image which is described in Sections 5.1 and in Appendix B.
>> Fetch which is used to FTP files to and from other computers

In the Applications Folder:

>> Spyglass is described in Appendix C. This program permits the plotting of 2D data in a Contour Plot format as well as in a 3D format.
>> ClarisDraw is a complete plotting program with extensive drawing tools and features. It is useful in combining multiple SANS images (imported from SANS Image by cutting-and-pasting) into the same page along with legends and comments. This page can then be plotted at the instrument using the DeskJet printer.
>> Kaleidagraph is useful for plotting averaged data in a X,Y format for example.
>> Adobe Acrobat used to convert data formats.
>> Igor software to plot reduced SANS data and to do nonlinear least squares fitting to a number of available functional forms.

The following application softwares have been installed on the PCs running Windows NT:

>> Microsoft Office (Word, Access, Excel, etc)
>> Netscape Communicator
>> Adobe Acrobat Reader
>> Ws_FTP to tranfer files to dikettes or to zip drives
>> TeraTerm (terminal emulator) to connect to the MicroVax.

APPENDICES

APPENDIX A: The RPA Equation

The **FIT/RPA** program uses the following Random Phase Approximation equation (so called de Gennes formula) for binary polymer blends of hydrogenated (H) and deuterated (D) polymers:

$$\frac{K_N}{\frac{d\Sigma}{d\Omega}(Q)} = \frac{1}{N_H V_H \phi_H D(QR_{GH})} + \frac{1}{N_D V_D \phi_D D(QR_{GD})} - \frac{2\chi}{V_0}$$

where the R_G's are the radii of gyration,

$$R_{GH} = \sqrt{\frac{N_H a_H^2}{6}} \; ; \; R_{GD} = \sqrt{\frac{N_D a_D^2}{6}}$$

the a's are the segment lengths, and D(x) is the Debye function for the structure factor of random coils,

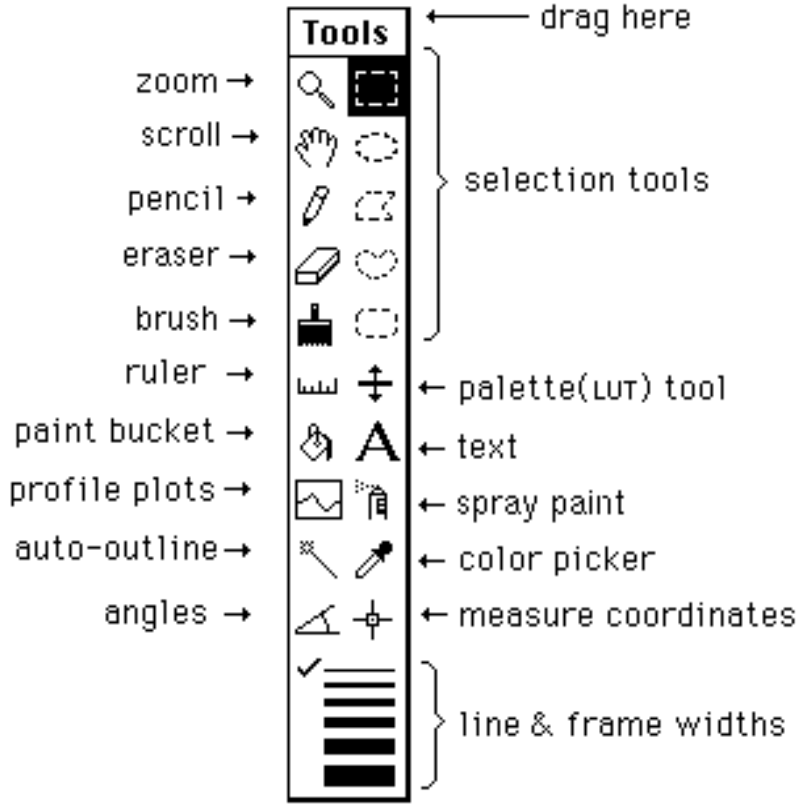
$$D(x) = \frac{2(e^{-x} + x - 1)}{x^2}$$

where $x = (QR_G)^2$. The N's are the degrees of polymerization, the V's are the monomer specific volumes, and the ϕ's are the volume fractions. χ is the Flory-Huggins interaction parameter and K_N is the contrast factor. A description of the **RPA parameters** for the **B and C polystyrene standards** can be found in **Table 3**.

APPENDIX B: SANS Image Drawing Tools

B.1 Description of Tools

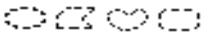
A diagram of the **SANS Image** tools and a short description of each is provided below. The window containing the tool palette can be moved to any location on the screen.



Magnifying Glass - Click within the active image window to zoom. Double-click on the magnifying glass to unzoom. OPTION-click (or use Undo) within the image window to unzoom in steps. Notice how the plus sign changes to a minus sign when you hold the OPTION key down.

Scrolling Tool (Grabber) - Moves images within windows. When using other tools, with the exception of the text tool, you can temporarily switch to the grabber by holding down the space bar.

Selection Rectangle - Use this tool to specify a rectangular subregion for use by commands in the EDIT, FUNCTIONS and ANALYSIS menus. Rectangular selections can be SAVED, COPIED, FILLED, CLEARED, INVERTED, FRAMED, FILTERED, or MEASURED. Hold down the SHIFT key to constrain the selection to be square. Double-click to select the entire image. As the rectangle is being drawn, its width and height are shown in the RESULTS window.



Oval, Polygon, Freehand, Rounded Rectangle - These are outlining tools for defining non-rectangular subregions for use by various commands in the EDIT, FUNCTIONS and ANALYSIS menus. Regions defined by these tools, along with the rectangle tool, can be SAVED, COPIED, FILLED, CLEARED, INVERTED, FRAMED, FILTERED, or MEASURED. The FILL command allows you to change colors after a region has been filled by clicking in the LUT window. Similarly, DRAW BOUNDARY allows you to change the line width by clicking on the lines in the Tools window. Double-click on the polygon tool to bring up the Measurement Options dialog box. Use the arrow keys to “nudge” selections one pixel at a time.

Pencil - Draws thin lines using the current foreground color. OPTION-click to pick up the color under the pencil. This works in either the current image window or the LUT window. It is not necessary to hold down the OPTION key to pick up colors from the LUT window. Holding down the SHIFT key causes pencil movements to be constrained to be either horizontal or vertical.

Eraser - Erases to the current background color. OPTION-click to pick up background colors from within the image window. The eraser can also pick up background colors from the LUT window. Holding down the SHIFT key causes eraser movements to be constrained to be either horizontal or vertical. The color of the eraser indicates the current background color. The background color is used by the CUT and CLEAR commands and as the background color for text. Double-click on the eraser to erase the active image window.

Paint Brush - Draws in the current foreground color. OPTION-click to pick up the color under the brush. It is not necessary to hold down the OPTION key to pick up colors from the LUT window. The color of the brush indicates the current foreground color. Double-click on the brush to change its size. Holding down the SHIFT key causes brush movements to be constrained to be either horizontal or vertical.

LUT Tool - This tool is used to dynamically modify the color look-up table (LUT) by clicking and dragging in the LUT window. It is also used to manipulate the density slice when thresholding is enabled. Double-click on this tool to enable/disable thresholding.

Airbrush Tool - Double-click to change the brush diameter.

Ruler - Draws straight lines and measures linear distances. To measure a distance (or draw a line), click at the starting point, drag to the ending point, and then let the mouse button up. The horizontal distance (X), vertical distance (Y), and total distance will be dynamically shown in the RESULTS window as the line is drawn. If you are measuring, and don't want to leave the line as a reference, use the UNDO (Command-Z) to erase it.

Hold down the OPTION key to measure distances along an irregular path. Terminate tracing by double clicking. It is only necessary to hold the OPTION key down at the start of tracing.

Lines can be constrained to be either vertical or horizontal by holding down the SHIFT key. Line width is specified by clicking on the lines at the bottom of the Tools window. Distances are given in pixels unless SET SCALE has been used to perform spatial calibration. Use SHOW RESULTS to display length measurements. Double-click on the ruler to bring up the Set Scale dialog box.

Wand (Auto-Outline) Tool - Double-clicking on the Wand tool highlights a portion of the color LUT and the portion of the data which corresponds to it. This is known as thresholding and is useful for defining a data region in order to locate the beam center (as described in Section 5.1.3). The highlighted data region can be manipulated by clicking and dragging in the thresholded region in the LUT.

Density Profile Tool - Displays a plot of the scaled data values along an arbitrary line. You generate this line in the same way you use the ruler tool to draw lines or to measure lengths. Hold down the OPTION key if you want the line drawn for reference purposes. Averaging will be performed if the line width is greater than one. For example, assume the maximum line width is selected by clicking on the thickest line at the bottom of the tool palette, then each data point plotted is the average of eight pixels. The PLOT window, unlike the HISTOGRAM window, may be resized. Lines can be constrained to horizontal or vertical be holding down the SHIFT key.

Plots can be copied to the Clipboard and then pasted into a picture window. In addition to the plot, the COPY command also copies the plot data to the clipboard as a single column of numbers, where it can be pasted into analysis and plotting programs.

Paint Bucket - This is a MacPaint-like Paint Bucket. It causes all pixels located where paint can leak from the starting point (the end of the paint coming from the bucket) to be changed to the foreground color. In conjunction with density slicing, it can be used for measuring areas under profile plots. Profile plots must first be pasted into an image window before they can be filled using the Paint Bucket.

Text Tool - When only words will do. Allows typing in the FONT and STYLE chosen in the appropriate menus. Various attributes of the text, such as font, size and color, can be changed after the text has been entered, but once another tool has been chosen, or you have typed RETURN, the text becomes part of the image's bitmap.

Hold down the OPTION key and the text tool will automatically type for you the most recent area measurement. If you prefer, it will enter the most recent mean density reading if you use MEASUREMENT OPTIONS to disable area measurements. Repeated option-clicking will enter previous readings, starting with the most recent one.

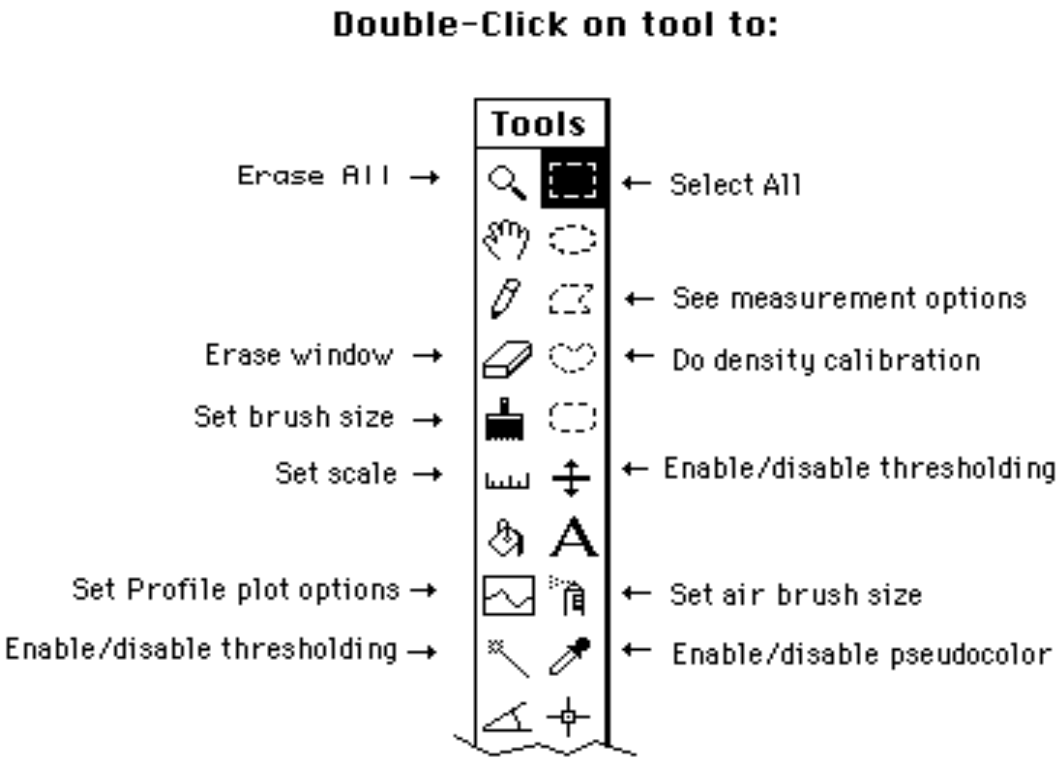
Eyedropper - Picks up colors from the active picture window and from the LUT window. Option-click to pick up background colors. If you are using pseudocolor, double-clicking on a color in the LUT window causes the Color Picker dialog box to be displayed, allowing you to modify that color. Double-clicking in the LUT window also allows you to change the density slice color when Image is in the density slicing mode.

Angle Tool - Measures the angle formed by two lines drawn through a point by this tool. The value is shown interactively in the RESULTS window. UNDO can be used to delete the lines if they are not wanted.

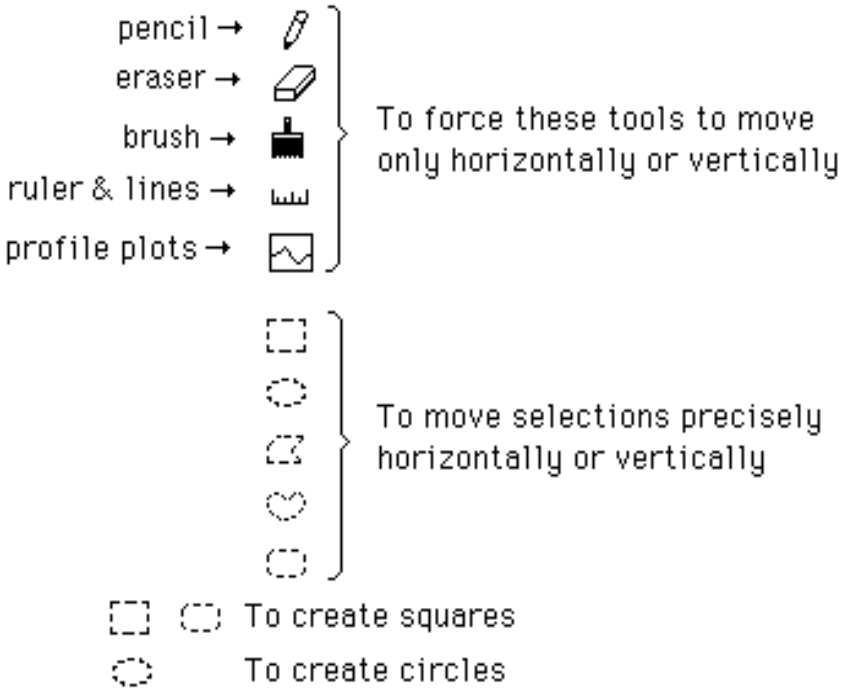
Counting Tool - Counts objects and records their X-Y coordinates, leaving markers so that objects are not counted twice. Markers are drawn in the current foreground color and their size is related to the current line width. Use the SHOW RESULTS command to display the X-Y coordinates.

Line Width - Allows user to choose the line width used by the ruler and profile plot tools and by the DRAW BOUNDARY command. The lines are 1, 2, 3, 4, 6, or 8 pixels in width.

B.2 Tool Shortcuts



To constrain tool functions hold down the shift key:



APPENDIX C: Using SPYGLASS Transform to Visualize SANS Data

SPYGLASS Transform can be used to create various useful graphical displays of SANS data, such as 2-D color images, 2-D contour plots, and 3-D surface plots. It is an easy-to-use Macintosh application which can help highlight particular features in the data, and provide color outputs (including transparencies).

Using SPYGLASS Transform generally requires (i) reducing the data in your SANS account on the MicroVax, (ii) transporting the data from the MicroVax to a Macintosh computer, and (iii) importing the data into the SPYGLASS environment. Data reduction should follow your typical scheme; i.e. appropriate application of the ADD, COR, DIV, and MASK programs. (A mask should be applied which, at the very least, removes the "unreliable" border pixels from the data image). For easiest use of SPYGLASS, the format of your final WORK file must be changed to ASCII using the program ASCII[1].

The next step is to transport the ASCII data from the MicroVax to your Macintosh. There are various ftp-type programs available to do this. For example, both FETCH and NETCOPY are easy to use for Mac users and should be on all of our Macs. Once the data file is transported to a Mac folder it can be retrieved and imported into SPYGLASS. Start by opening the SPYGLASS Transform application (by double clicking on the SPYGLASS Transform icon). To import SANS data, scroll under the MACROS menu heading, and choose the MACRO entitled SANS_ASCII_64x64. This MACRO will ask you which file to open and then does the following operations: (i) it imports the data into a SPYGLASS data table, (ii) it creates a 2-D color image, (iii) it creates a surface plot, and (iv) it draws a contour plot of the log of the (normalized) data[2]. Each of these plots can be modified to your liking, for example by "fiddling" with the color, changing the axis, re-scaling the plot size, or changing the contour levels. To familiarize yourself with these features, you can use the SPYGLASS Transform manuals which are available in the computer room. Finally, images can be printed on any of the available printers. To change to a color printer use the CHOOSER menu and select the HP appropriate (NG3 or NG7) DeskJet printer.

Notes:

1.) SPYGLASS Transform can also handle binary data formats. For example, the data transfer procedure from the MicroVax to the Macs can be replaced by using VIEW/WORK, which transfers your WORK file in a binary format. To utilize this, you would then use the SPYGLASS MACRO (see below) entitled SANS_VIEW_128x128. The only disadvantage to this is there may be a loss of resolution since VIEW/WORK compresses the intensity data to values between 0 and 256.

2.) If you want to import data into SPYGLASS Transform without using the MACRO's, the following are used:

(i) for ASCII -- Open using "Text Matrix"; lines to skip = 17, rows = 64, cols = 64.

(ii) for binary data transferred using VIEW -- Open using "Binary Matrix"; unsigned 8-bit, lines to skip = 0, rows = 128, cols = 128.

TABLES

Table 1: List of Available Absolute Standards

Standard Name	Cross Section (cm^{-1})	Thickness (mm)	R_g (A)	Trans @ 6A	Q-Range (A^{-1})	Program
Sil A1	25.7	1	30.8	.90	.02-.04	FIT
Sil A2	27.9	1	30.8	.90	.02-.04	FIT
Sil A3						
Sil A4						
Sil A5	23.7	1	30.5	.930	.02-.04	FIT
Sil A6	22.3	1	31.1	.923	.02-.04	FIT
Sil A7	22.4	1	30.8	.918	.02-.04	FIT
Sil A8	23.7	1	30.8	.910	.02-.04	FIT
Sil B1	56.6	1	58.0	.92	.01-.025	FIT
Sil B2	54	1	58.3	.92	.01-.025	FIT
Pol AS1	65.7	1	75.3	.43	.01-.03	FIT/RPA
Pol AS2	63.8	1	76.1	.43	.01-.03	FIT/RPA
Pol B1	220	1.53	110	.56	.005-.03	FIT/RPA
Pol B2	220	1.53	110	.56	.005-.03	FIT/RPA
Pol C2	650	1.53	195	.55	.003-.03	FIT/RPA
Al-7	199	10.0	216		.003-.014	FIT

Use the FIT program (Guinier plot) for the Sil standards and FIT/RPA for the polymer standards. For the polymer standards, FIT/RPA yields a segment length of b=6.7 A (polystyrene).

NOTE: The values given for $d\Sigma(0)/d\Omega$ and the radius of gyration R_g (or the segment length b) are good to within ±5%.

Table 2: Absolute Cross Section for 1 mm Water.

Water is used as a standard if $Q_{min} > 0.02\ A^{-1}$.

Wavelength (A)	5	6	7	8	9	10	12	15
Cross Section (cm^{-1})								
Measured at NIST:	0.88	0.96	1.01	1.10	1.19	1.33	1.47	1.77
Measured at ILL:	0.83	0.86	0.89	0.92	0.94	0.97	1.03	1.11

Slight detector sensitivities cannot explain the difference between these two measured sets.

Table 3: Parameters Used by the FIT/RPA Program for the B and C Polystyrene Standards

Parameter	Value	Description
K_N	4.114×10^{-3} mole cm^{-4}	Contrast factor
V_H	99.52 cm^3 $mole^{-1}$	Molar volume of H-mer
V_D	100.36 cm^3 $mole^{-1}$	Molar volume of D-mer
V_0	99.94 cm^3 $mole^{-1}$	Average molar volume of blend
χ	1.1×10^{-4}	Interaction parameter

Parameter	B Std	C Std	Description
d	0.153 cm	0.153 cm	Sample thickness
N_H	1872	4993	H-mers/chain
N_D	1556	3937	D-mers/chain
ϕ_H	0.516	0.516	Volume fraction of H
$d\Sigma(0)/d\Omega$	220 cm^{-1}	650 cm^{-1}	Forward scattering cross-section

FIGURES